New atomic data portal

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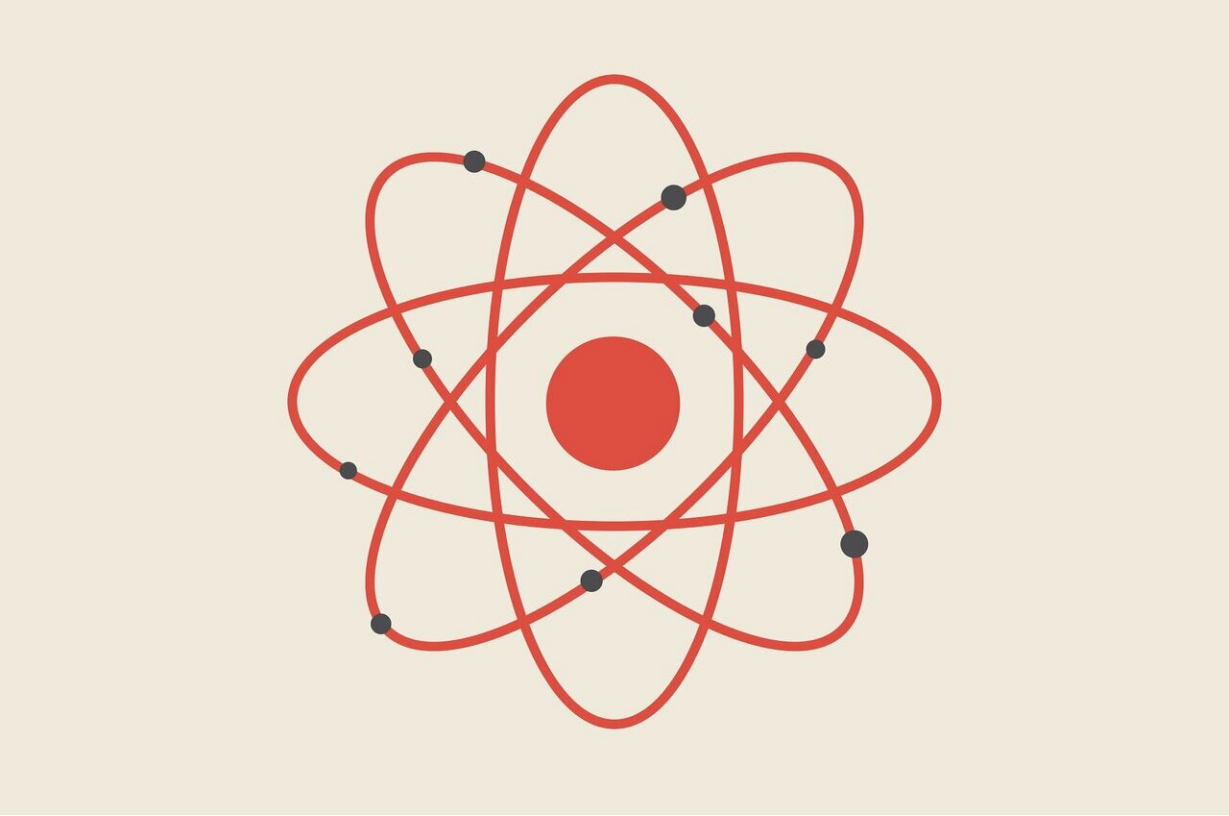

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Even if you're one of the most precise physicists on the planet—as University of Delaware Professor Marianna Safronova is—you still will need collaborators whose skills complement your own and make new opportunities possible.

You will need someone such as UD Professor Rudolf Eigenmann, who can take that precision, add generous amounts of computer science expertise and help to make that high-value information available to any other physicist who wants it.

A project led by Safronova and Eigenmann and supported by the National Science Foundation has done just that, producing a Portal for High-Precision Atomic Data and Computation that provides extraordinary information about atomic properties in user-friendly ways.

It's the periodic table on steroids and it is already drawing keen interest from researchers who need to know the nitty-gritty details of the materials they work with.

"The properties are key inputs for many research projects, such as quantum simulation, development of quantum sensors, tests of fundamental physics and many others," Eigenmann said. "Atomic data are important for astrophysicists and plasma physics applications and may help to shed light on how heavy elements such as gold and uranium are produced in the universe."

Bindiya Arora, a UD alum who now is a physics professor at Guru Nanak Dev University (GNDU) in Punjab, India, worked on the fundamental physics and modeling with Safronova. Eigenmann, computer engineering graduate student Parinaz Barakhshan and physics graduate student Adam Marrs developed the computer mechanisms and interfaces that put the calculations to work.

Knowing the precise atoms in materials is of critical importance in engineering characteristics and science projects. Now a growing body of high-precision data is available online, giving the research community a new power tool for a broad range of applications in physics and engineering.

Safronova's calculations already have contributed to many such advances, including the development and fundamental research with optical atomic and nuclear clocks, tests of fundamental symmetries, studies of dark matter and other projects that are pushing past standard particle physics models.

"Our group and collaborators have developed high-precision code over the past 20 years," Safronova. "This portal makes them searchable and easy to access. In many cases, those properties have not been measured before. This data is not provided by any other database."

The new portal provides access to calculations of properties of atoms and ions, such as matrix elements, transition rates, lifetimes, polarizabilities, hyperfine constants and others.

The computer science challenge included finding efficient ways to link Safronova's complex computations with an online portal that could automatically include new data.

The first version of the portal included data on 12 elements. Already, scientists and engineers have asked for more. Safronova said the hope is to add 30 more elements in the next year.

The information can be used for fundamental physics, Safronova said, precision measurements, quantum simulation, atomic clocks and astrophysics, to name just a few applications.

"You may wonder why we can provide this information at the University of Delaware and others can't," Eigenmann said. "The previous work of Marianna and her collaborators has created these computational techniques that produce precision no one else has."

The portal is open to all and free to use. And, Safronova said, it would

not exist without the help of Eigenmann and his team.

"I had no idea how to get that data online," she said. "I know how to produce the data and I know how to publish the numbers. But to make a website and release actual codes—I had no idea how to do that. Collaborating with computer scientists taught me so much about how I should write code. We redesigned a lot of codes to make more of the software."

Marrs said the project has been a good challenge for him, too.

"The collaboration forced my brain to go in two different ways," he said. "It was very much a learning process. High precision numbers I'm familiar with. But doing it in this way, where we want it to be seen by everyone, motivated me to make the whole process as automatic as possible."

Arora said she knew from previous studies that Safronova knew how to produce precision code. But Arora had never worked on converting those codes for open access.

"Compiling data from various experiments is part of my job, and this gave me insight to new findings," she said. "All the complicated codes and software were available, but they were very hard to use. The kind of open access we are trying to provide is easy to use. You just need to know what kind of atom you want and what property you want to work on."

Safronova said the work was done using UD's high-performance Caviness and Darwin clusters.

"This code requires high-performance computing," she said.

That means far more muscle than an ordinary computer can muster. Darwin has 6,000 cores available—the approximate capacity of 6,000 computers. Safronova's team uses more than 500 cores.

And that powerful computation now is available to those who may not have HPC skills or access. The portal is web-based, available to anyone with an Internet connection. Eigenmann said it could one day be accessible with a mobile app.

That could put the power of the Darwin computations into many a pocket.

"This collaboration has been rewarding on all sides," he said. "I enjoy learning physics and some of it takes me back to high school and the periodic table. What we do in computer science—I find it rewarding when we see the application in physics, biology or chemistry. There are interesting computer science issues there."

Provided by University of Delaware